A new hybrid Lagrangian numerical scheme utilizing phase space grid for XGC1 edge gyrokinetic code

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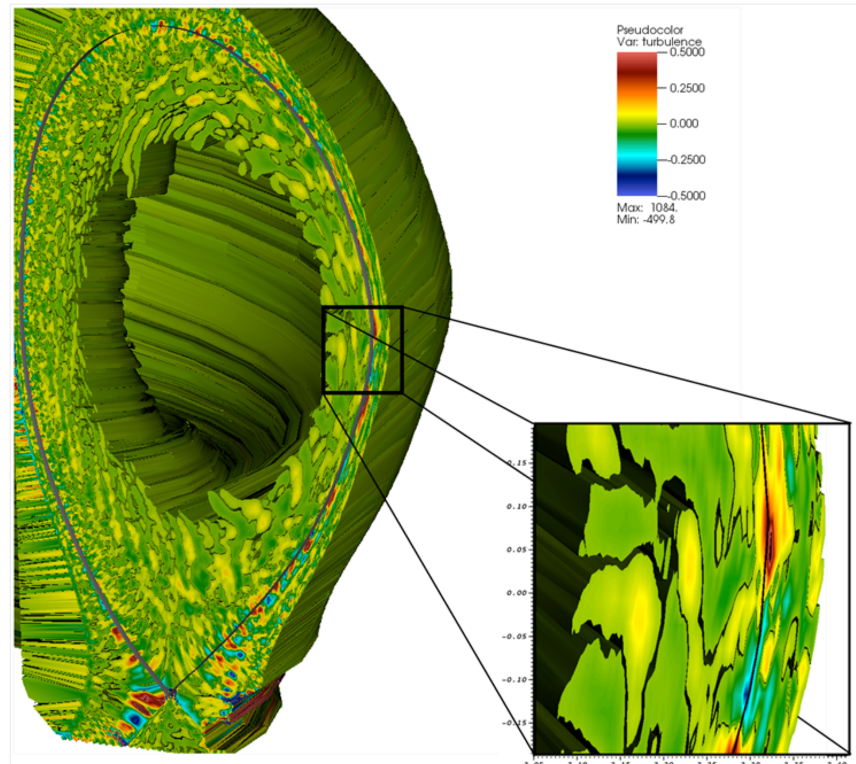
Outline

- Tokamak edge plasmas and XGC1
- Total-f (full-f), conventional δf, and total-δf PIC
- New hybrid Lagrangian scheme
  - Needed for edge simulation (reduces weight-growth from wall-loss, enables non-linear collision)
  - Use both particle and v-space-grid
  - Direct weight evolution
  - Used in XGC1/a for all physics
- Example in a simple ITG turbulence case
  - The α-factor and numerical dissipation
  - Homogeneous marker distribution in v-space

Tokamak Edge Plamsas

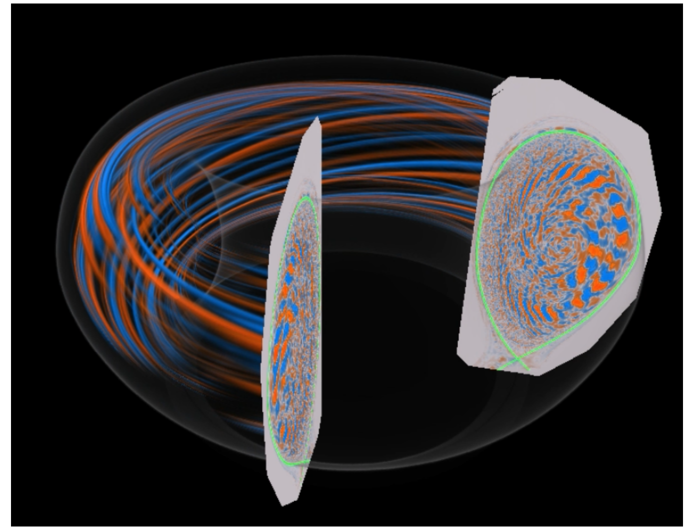
- Non-Maxwellian
  - Steep H-mode gradient
  - In-contact with wall
  - Strong turbulence level ($\delta n/\langle n\rangle \sim 10\%$)
- Sources and Sinks
  - Wall loss
  - Neutral atoms
  - Radiative cooling

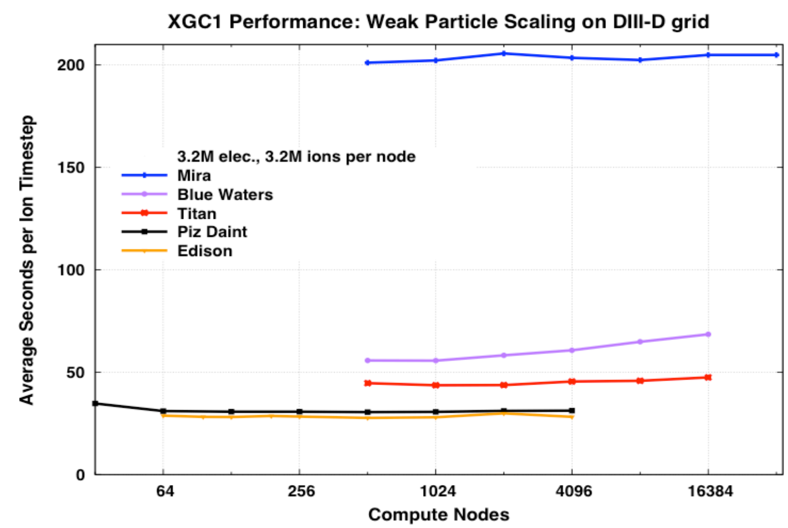


XGC1: X-point included Gyrokinetic Code

- Uses experimental EFIT data
  - Magnetic fields
  - Divertor and limiter
- Fully nonlinear Fokker-Plank – Landau collision on v-space grid
- Logical sheath to handle wall boundary
- Built-in neutral Monte-Carlo routine and atomic cross sections

- GPU+CPU hybrid capability
- Good weak and strong scaling to maximal capability of the leadership HPCs (titan, mira, and edison).





PIC simulation of Tokamak plamsas: Total-f vs conventional δf

- Total-f (Full-f): Solve f directly without manipulation
  - $Df/Dt = C(f) + \text{Source} - \text{Sink}$
  - Original XGC1
- Conventional δf in Tokamak plasmas
  - $f = f_0$(fixed analytically) + δf
  - $\dfrac{D\delta f}{Dt} \cong -\dfrac{D^* f_0}{D^* t} + C = -v_E \cdot \nabla f_0 + C$
  - No neoclassical (grad-B drift) free energy on RHS
  - Scale separation between mean (f_o) and perturbed δf is assumed
  - Main plasmas in most of core δf codes

Total-δf particle methods

- Total-δf
  - $f = f_0 + \delta f$

$$\frac{D\delta f}{Dt} = -\frac{Df_0}{Dt} + C + \mathrm{Source} - \mathrm{Sink}$$

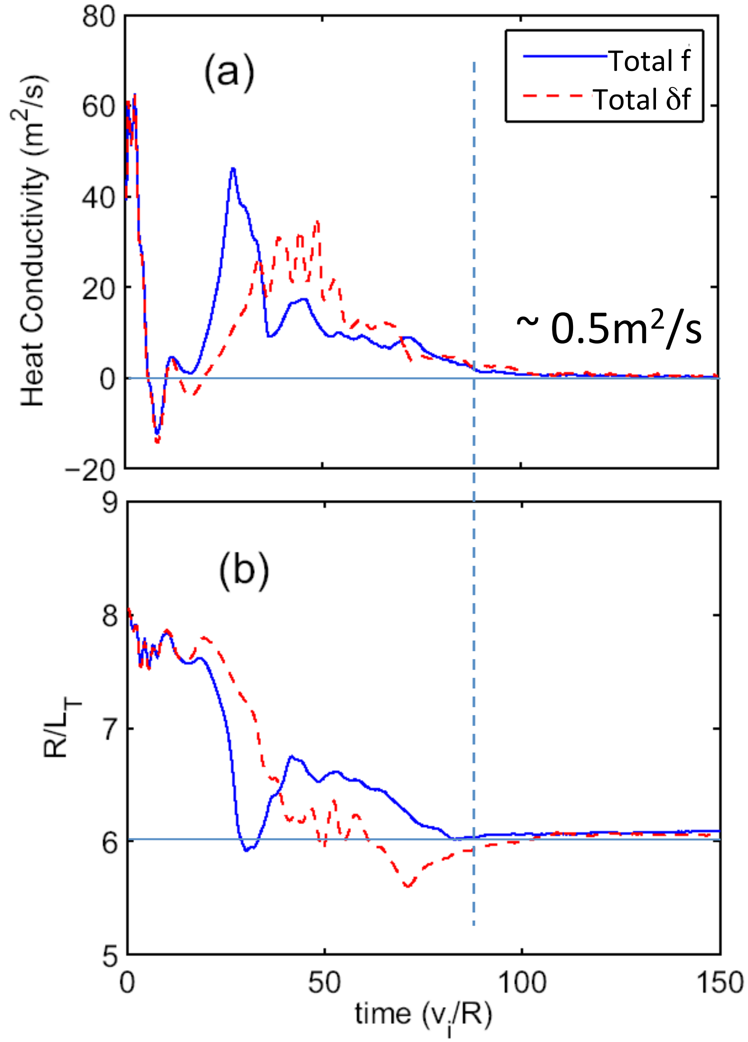
  - **D/Dt contains all physics**
  - **Mathematically identical to total-f**
  - Mean and perturbed physics are solved together
  - Includes sources and sinks
  - δf can can become large due to strong neocalssical drive, wall loss, sources, or long time evolution.

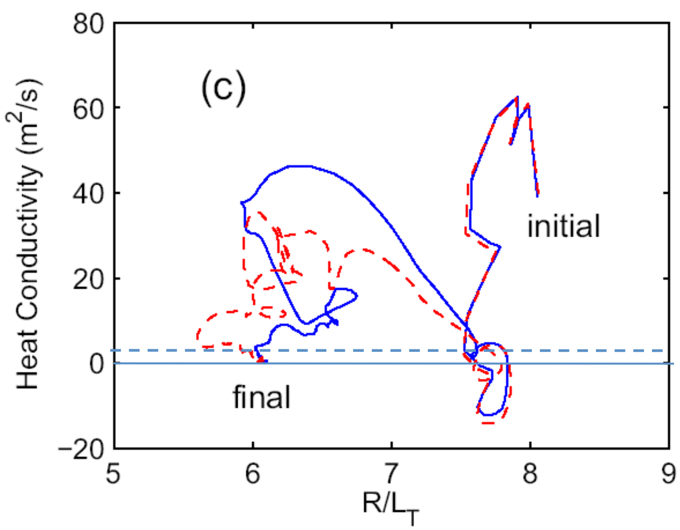
    → Growing weight and noise problem
  - Difficult to handle wall loss and non-linear collision

Comparison between total-f and total-δf

[Ku et al., Nuclear Fusion 2009]

- Non-flux driven→ solutions decay
- Transient behavior is different, caused by the different Monte-Carlo noise level, but time integrated heat flux is the same
- Meaningful steady state solutions agree.





New hybrid Lagrangian scheme

- Solve total-δf eq.
- $f = f_0 + f_P = f_a + f_g + f_P$, enables edge simulation
- f_0 contains slowly varying physics in time.
- f_a is a fixed analytic distribution function (e.g. Maxwellian).
- f_g is deviation from f_a on 5D grid.
- f_P represents δf particles, driven by the free energy in f_a and f_g.
- All physics information on continuum grid, with f_p moved to v-grid.

f_a	f_g	f_p
Analytic function	V-space grid	Particles

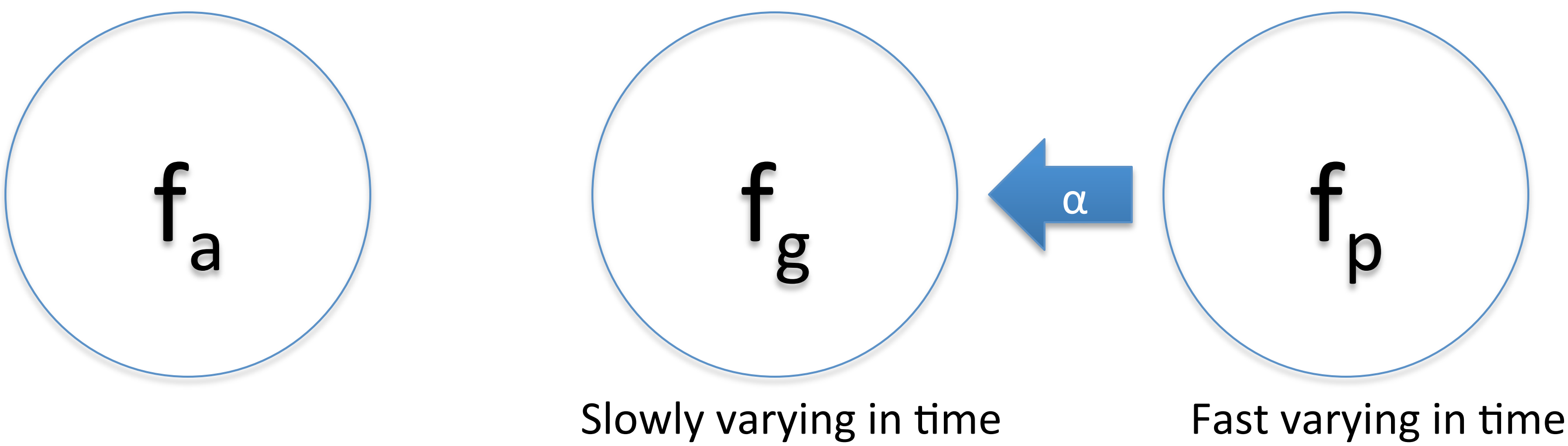
New hybrid Lagrangian scheme

- Time evolution:
  - Step 1 : Solve particle motion and weight evolution as in the total-δf scheme + S operation in v-grid

$$\frac{Df_P}{Dt} = -\frac{D(f_a + f_g)}{Dt} + S(\text{v-grid})$$

  - Step 2 : Redefine f_P and f_g with the following operation (α<<1)

$$f_P \Leftarrow [1-\alpha(X,V)]f_P \;, \quad f_g \Leftarrow f_g + \alpha(X,V) f_P$$



Direct weight evolution

- Gyrokinetic Vlasov-Boltzman eq. $$\frac{Df_p}{Dt} = -\frac{Df_0}{Dt} + S(f)$$
- Differential form of weight evolution (2 weights, Hu and Kromess)

$$\frac{dw_1}{dt} = \frac{(1-w_2)}{f_0}\left[\frac{Df_0}{Dt} + S\right] \qquad \frac{dw_2}{dt} = \frac{(1-w_2)}{f_0}\frac{Df_0}{Dt}$$

  – Similar to Y. Chen PoP (1997) and W. Wang PPCF(1999) except for **deterministic particle motion** from continuum collision.

- **Direct weight evolution (new)**

$$\frac{(1-w_2)}{f_0} = \text{constant} \qquad \Delta w_1 = \Delta w_2 + S\frac{(1-w_2)}{f_0}\Delta t$$

  – **Maker particles conserve phase space density**
    - Unlike conventional δf: Due to inaccuracy in D*/D*t operation
  – Avoid w_2 errors from time integrator and D/Dt error from gradient

Weight evolution of wall loss

- Marker particle is reflected at wall
  - Elastic reflection
  - Conserve phase space volume
  - w_2 remains the same
  - cf. reflection by sheath potential
- f=0 with wall loss
  - Reflected marker particle cancels f_0

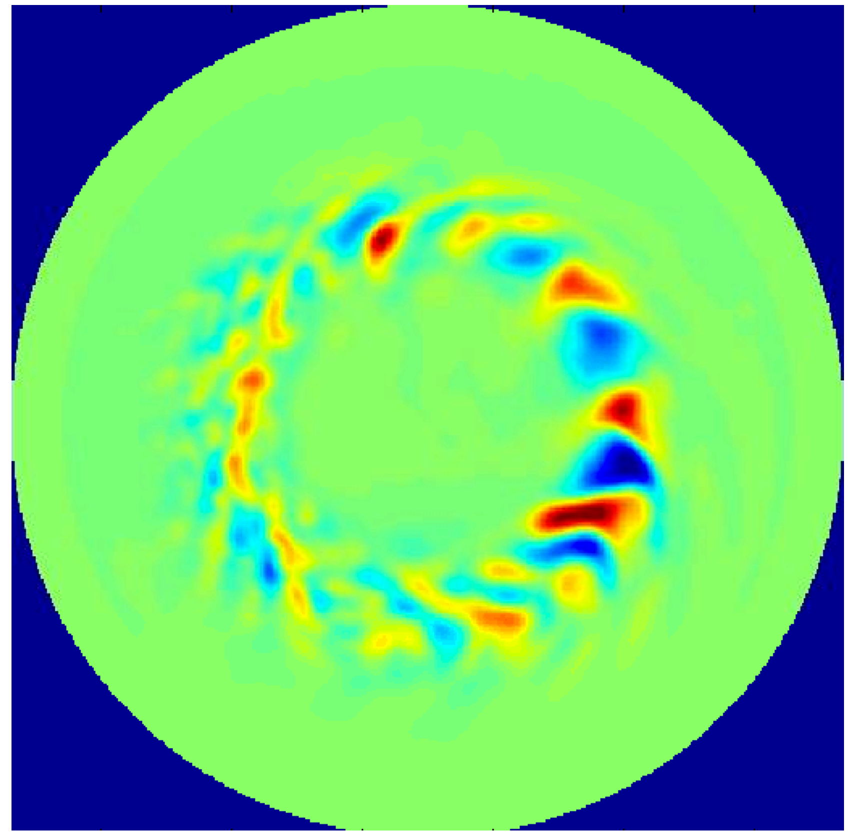
$$\boxed{w_1 = -1 + w_2} \longleftarrow \boxed{\begin{aligned} & f = f_0 + w_1 g = 0 \\ & (1 - w_2) g = f_0 \end{aligned}}$$

Advantage in continuum grid

- Weight reduction using v-space f_g
- Continuum space physics operation with f_p moved to continuum grid
  - **Nonlinear collision**
  - Neutral ionization and C-X
  - Radiation

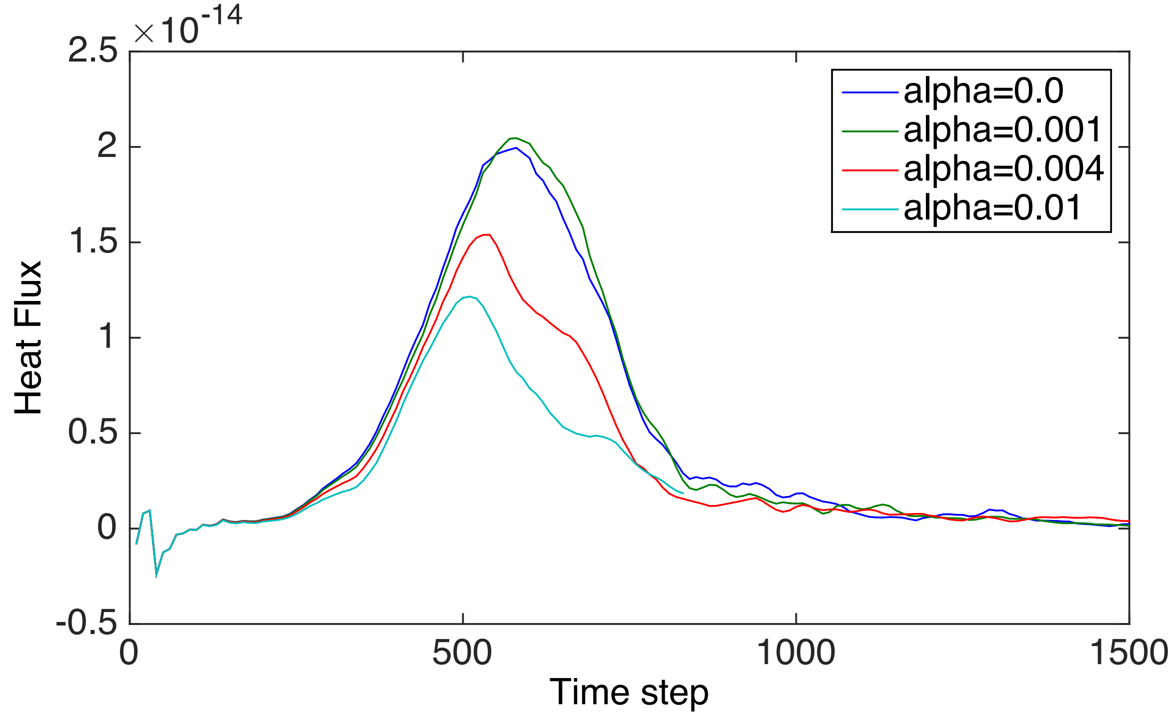
ITG turbulence in cyclone geometry

- Collisionless
  - Collision capability presented by R. Hager
- 0.3M real space grid
- 32 by 31 v-space grid
  - Slow physics on v-grid
- 400M particles
  - 1500 ptls/real space grid
  - 1.5 ptls/v-space grid
  - Fast physics in the particles



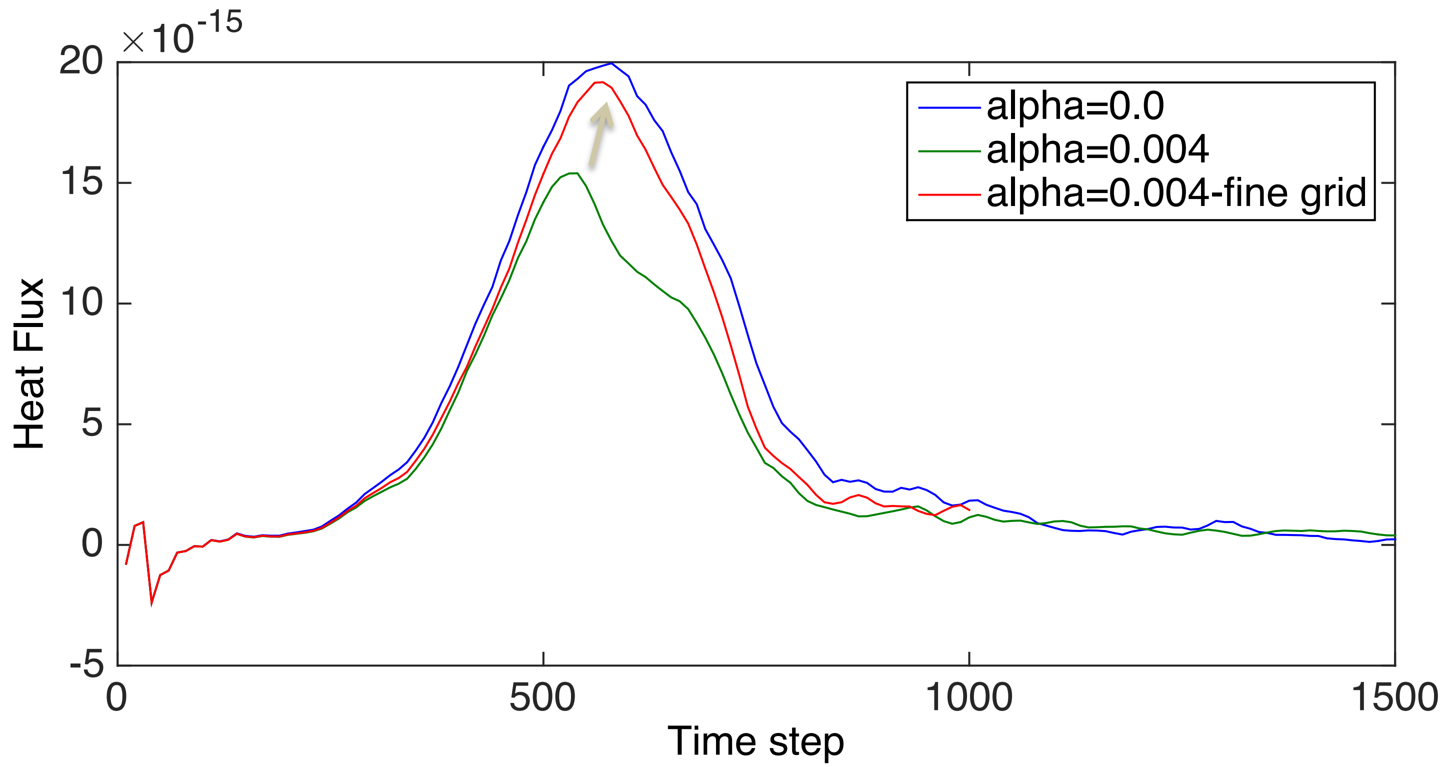
α factor and numerical dissipation

$$f_P \Leftarrow (1-\alpha) f_P$$
$$f_g \Leftarrow f_g + \alpha f_P$$



- Non-flux driven, total-deltaf
- Particle → v-space operation gives numerical dissipation from interpolation (damping of Landau resonance).
- Too large α reduces turbulence and time integrated heat flux
- Optimal α ~ C(Δv) Δt/[turbulence corelation time scale]

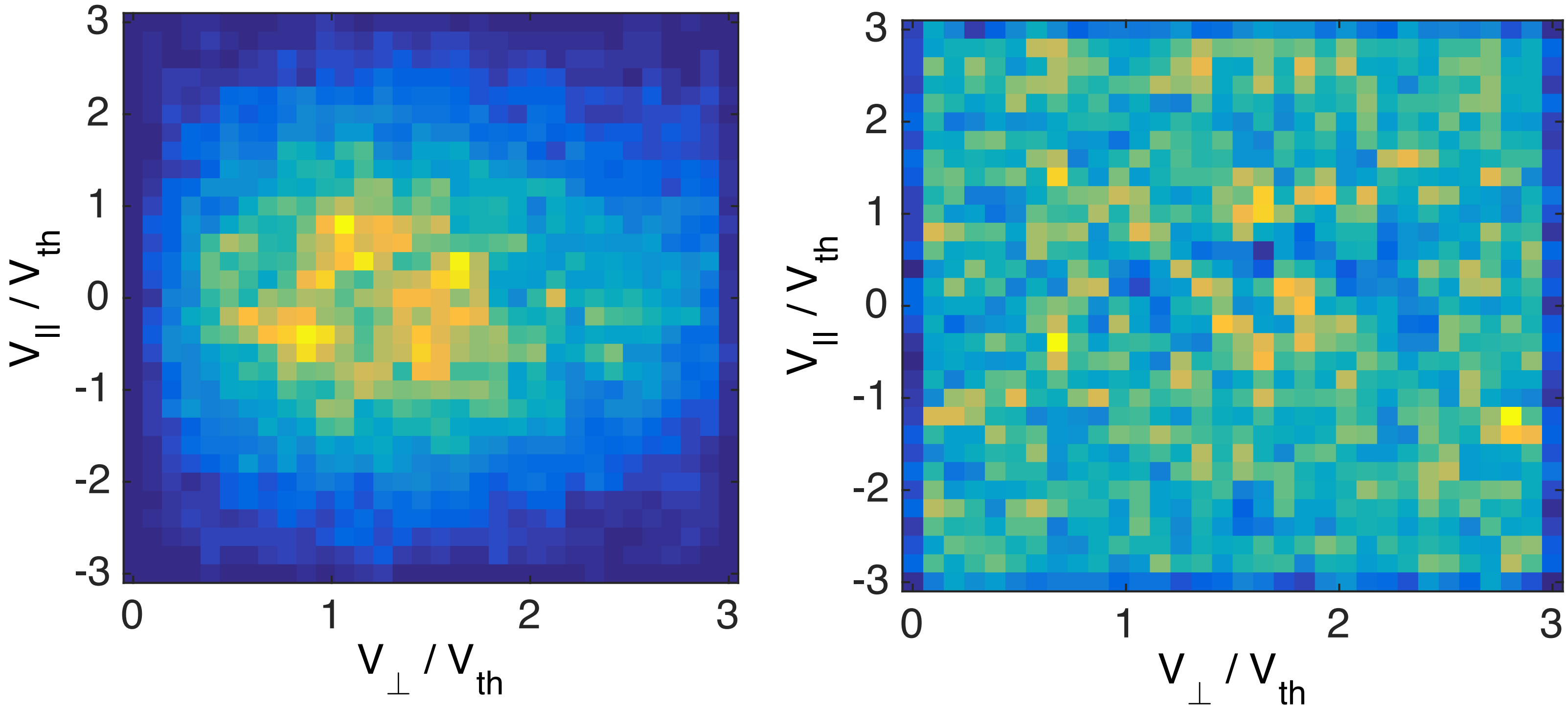
V-space grid resolution also matters



- Fine grid: v-space grid from 32 x 31 to 62 x 61
- Reduced numerical dissipation in v-space → restore original heat flux even at α = 0.004

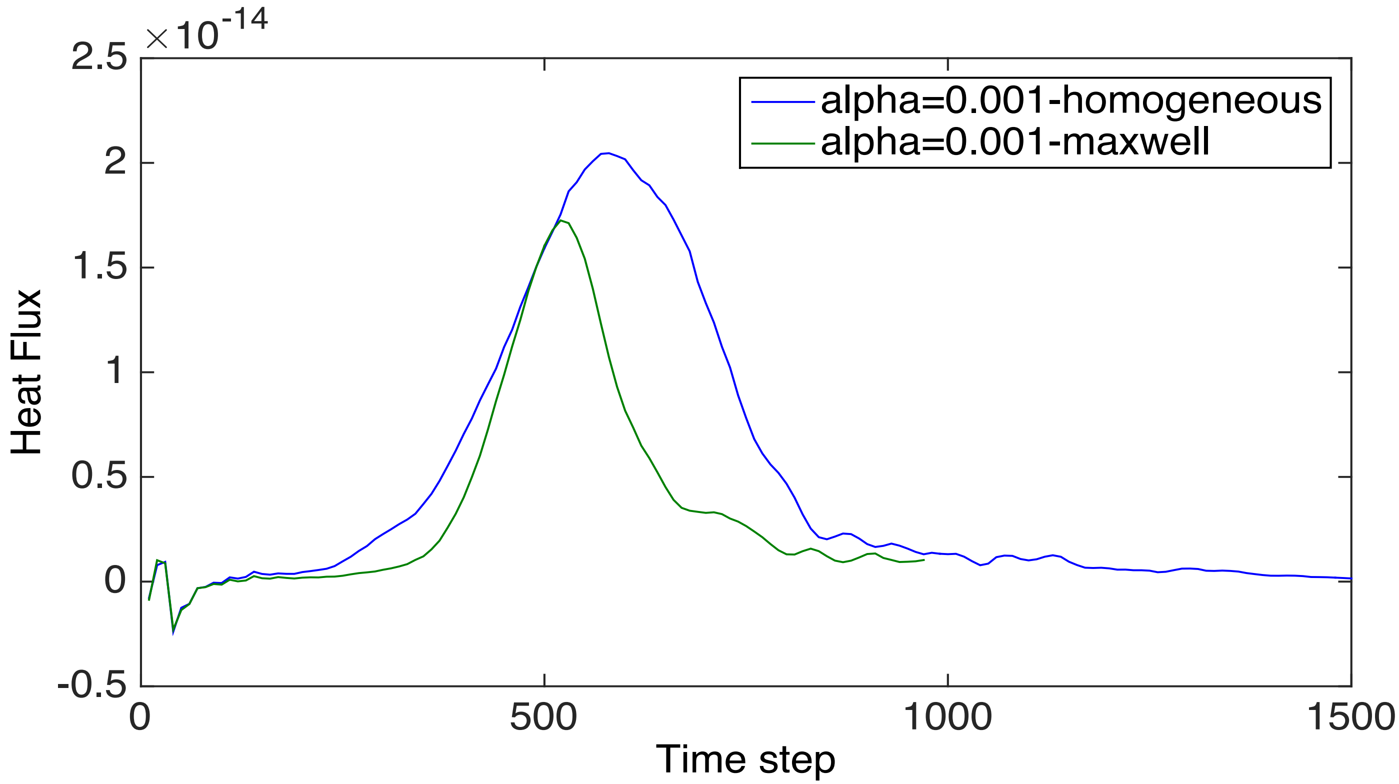
Homogeneous probabilistic marker initialization in v-space for better statistics at higher energy

Number of particles in v-space cells



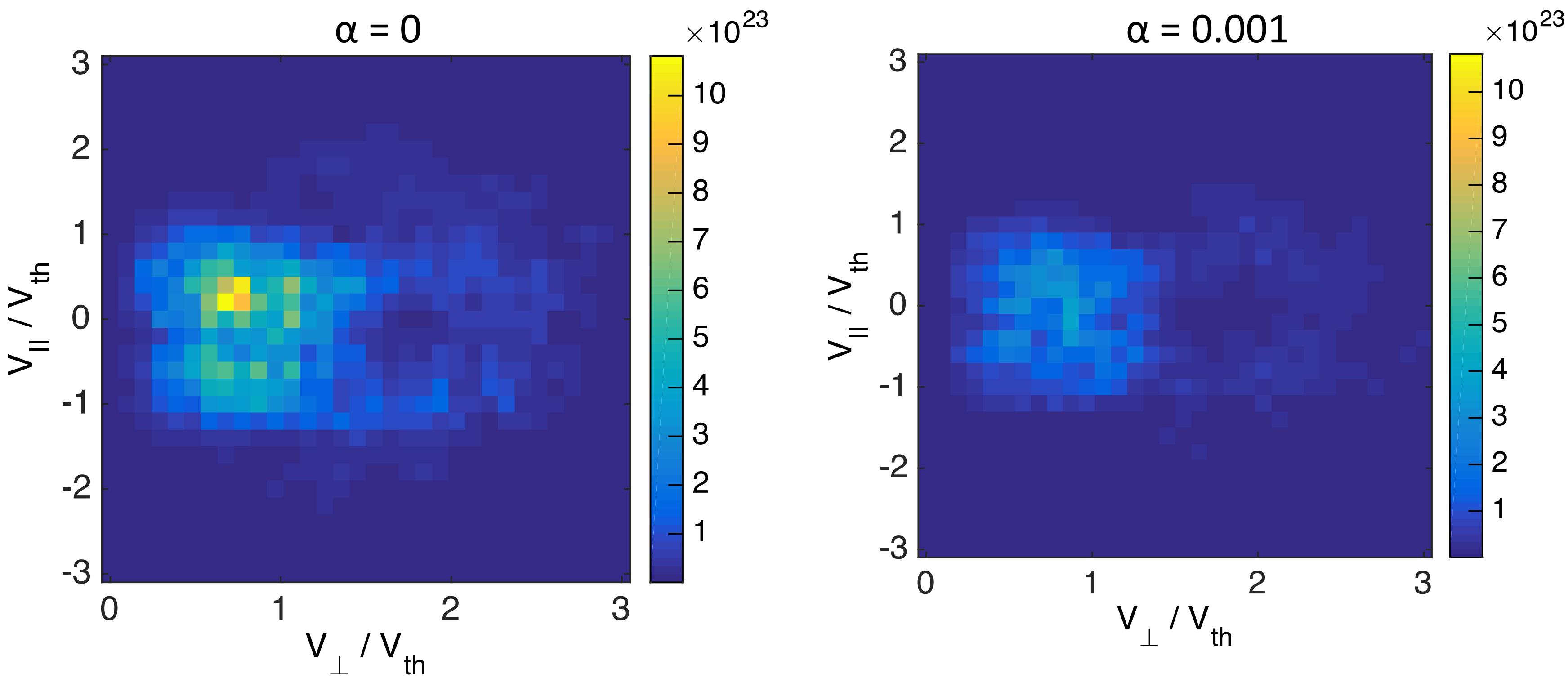
Maxwellian distribution   Homogeneous distribution

Homogeneous Marker distribution in v-space and greater # of particles can allow bigger α



- Homogeneous marker distribution gives better statistics
- Maxwellian distribution resembles less # ptls results

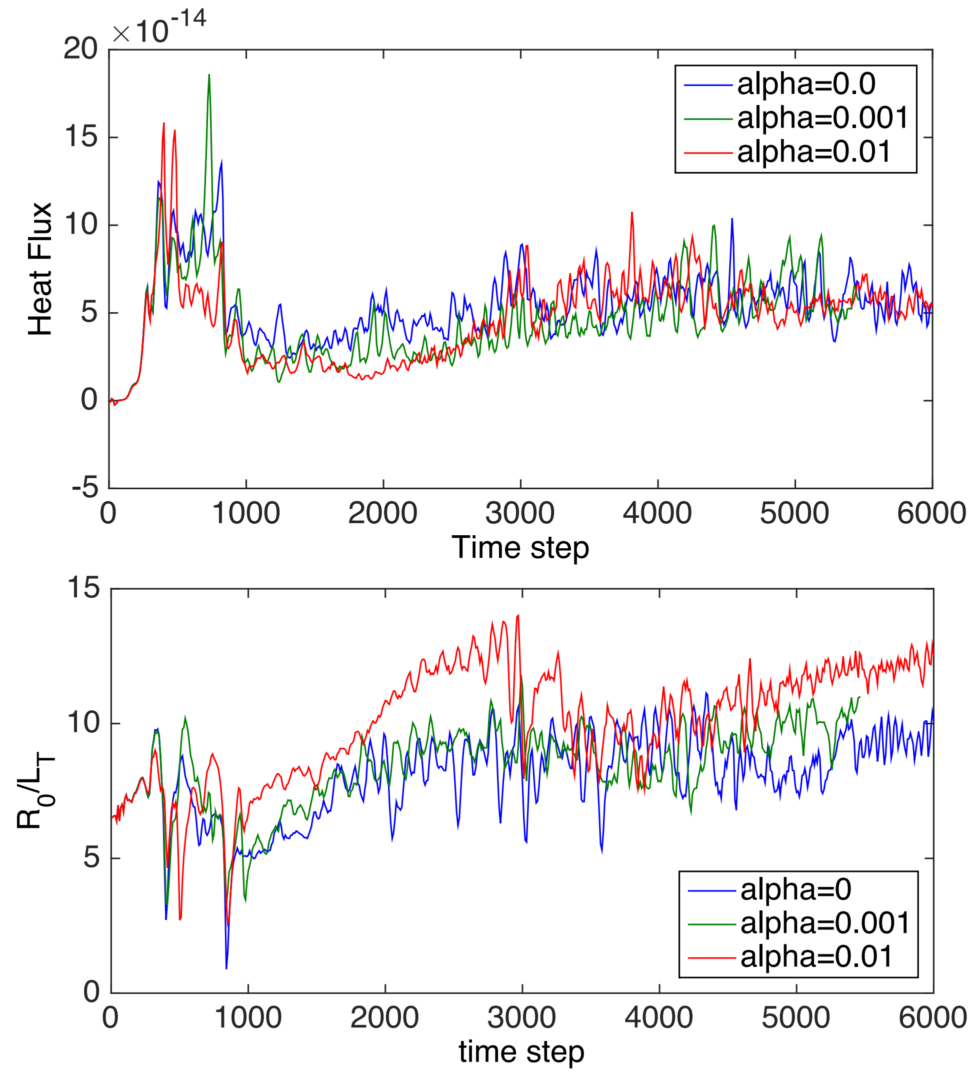
Particle Noise Reduction



- Variance of $w_1 g$ in v-space cell (g : Marker distribution)
- $\alpha = 0.001 \rightarrow$ reduce particle noise variance by 4 in 1500 time steps.
- Particle noise reduction

Flux driven simulation

- Heat and cooling is applied to near axis and edge
- Close to steady state
- α=0 and α=0.001 converges to similar gradient.
- Time integrated heat flux is different for α=0.01 from α=0.



Summary

- A new hybrid Lagrangian scheme for gyrokinetic simulation of tokamak edge plasma is implimented in XGC1.
  - Combination of particle and continuum
  - Lagrangian particle push
  - Difficult physics operation and noise reduction in continuum space
  - Direct weight evolution and homogeneous marker distribution help simulation accuracy
- The new scheme is equivalent to ‘total-f’ with
  - Sources and Sinks
  - Non-maxwellian distribution
- $f_{particle}$ is slowly converted to $f_{v\text{-}grid}$.
  - Slow time varying function → v-space grid
  - Fast time varying function remains in particles
  - Magnitude of α depends upon Δv and particle number.
  - The new scheme relaxes growing weight problem.